Normal Heat Conduction in a Chain with Weak Interparticle Anharmonic Potential

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We analytically study heat conduction in a chain with interparticle interaction $V(x) = \lambda[1 - \cos(x)]$ and harmonic on-site potential. We start with each site of the system connected to a Langevin heat bath, and investigate the case of small coupling for the interior sites in order to understand the behavior of the system with thermal reservoirs at the boundaries only. We study, in a perturbative analysis, the heat current in the steady state of the one-dimensional system with weak interparticle potential. We obtain an expression for the thermal conductivity, compare the low and high temperature regimes, and show that, as we turn off the couplings with the interior heat baths, there is a "phase transition:" the Fourier's law holds only at high temperatures.

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The understanding of heat conduction in a lattice system of interacting particles has become a challenging problem of statistical physics, even in the $1D$ context [1]. A central issue is finding a model Hamiltonian system for which Fourier's law holds. One of the first works in this subject was the (rigorous) study of the harmonic chain of interacting oscillators coupled to heat baths at the boundaries [2]. The authors show that the heat current is independent of the length of the chain, i.e., the Fourier's law does not hold. Since then, many (very often conflicting) works have been devoted to the problem, in particular, to investigations on the effects of nonlinearity and external potentials in the behavior of the heat current. We recall some results. In [3], the authors show that the conductivity is anomalous (i.e., it diverges) in any one-dimensional momentum conserving system, but in [4] and [5] a momentum conserving system with finite conductivity is presented. In [6], the authors claim that the anharmonicity of the on-site potential is a sufficient condition for a finite thermal conductivity, but in [7], it is shown to be wrong. Almost all the results are obtained by means of computer simulations, and, as emphasized in [8], besides the difficulty to arrive at correct conclusions from numerical studies, several works use the Green-Kubo formula for the conductivity, a formula which has never been rigorously established for this context. In short, more accurate studies are necessary.

In this scenario, the harmonic Hamiltonian chain of oscillators has been revisited quite recently [9], but for the case of each site connected to a thermal reservoir. The steady state is rigorously computed in the "self-consistent" condition, which means with no heat flow between an inner site and its reservoir. In such a model, the Fourier's law holds.

The present paper is addressed to the following issues: (i) the development of new analytical methods of modeling the heat conduction problem; (ii) the search for a system with normal conductivity and with, say, a small anharmonic potential (the problem which inspired the first investigation of Fermi, Pasta and Ulam [10]); (iii) the understanding of the temperature role on the thermal conductivity of chains with soft anharmonicity such as $V = 1 - \cos(q_{i+1} - q_i)$ (there is a recent debate, with positions against [11] and in favor of [12] a phase transition in the rotor model - i.e. finite thermal conductivity for large T, and infinite one for small T). Here, we extend the approach and techniques previously developed in [13] in order to treat a chain with thermal reservoirs at the boundaries only: now we consider different coupling constants among reservoirs and sites, and investigate the limit of the coupling with the interior heat bath taken to zero. Our approach is quite general, but we focus on the case of a chain of oscillators with a harmonic on-site potential and interparticle interaction $V = \lambda[1 - \cos(q_{i+1} - q_i)]$. We obtain (in a perturbative analysis) an expression for the thermal conductivity and investigate the Fourier's law: for our model, as we turn off the the couplings between inner sites and their reservoirs, it holds only at high temperatures.

Now we introduce the model. We consider the Langevin dynamics of an anharmonic crystal with stochastic heat bath at each site. Precisely, we start from N oscillators with Hamiltonian

$$H(q,p) = \sum_{j=1}^{N} \frac{1}{2}\left[p_j^2 + Mq_j^2\right] + \frac{1}{2}\sum_{j\neq l=1}^{N} \lambda[1 - \cos(q_l - q_j)], \tag{1}$$

($d = 1$ and next-neighbor interactions are assumed later) where $M > 0$, with time evolution, for $j = 1, \ldots, N$,

$$dq_j = p_j dt; \quad dp_j = -\frac{\partial H}{\partial q_j}dt - \zeta_j p_j dt + \gamma_j^{1/2} dB_j; \tag{2}$$

where B_j are independent Wiener processes; ζ_j is the heat bath coupling for the j^{th} site; and $\gamma_j = 2\zeta_j T_j$, where T_j is the temperature of the j^{th} heat bath.

As usual, we define the energy of the oscillator j as

$$H_j(q,p) = \frac{1}{2}p_j^2 + U^{(1)}(q_j) + \frac{1}{2}\sum_{l\neq j} U^{(2)}(q_j - q_l), \tag{3}$$

where the expression for $U^{(1)}$ and $U^{(2)}$ follow immediately from (1) and $\sum_{j=1}^{N} H_j = H$. Then, we get

$$\left\langle \frac{dH_j(t)}{dt} \right\rangle = \langle R_j(t)\rangle - \langle \mathcal{F}_{j\rightarrow} - \mathcal{F}_{\rightarrow j}\rangle\,, \tag{4}$$

where $\langle\cdot\rangle$ denotes the expectation with respect to the noise distribution, and

$$\langle R_j(t)\rangle = \zeta_j \left(T_j - \langle p_j^2\rangle\right) \tag{5}$$

gives the energy flux from the j^{th} reservoir to the j^{th} site. The remaining terms are related to the energy current inside the system and they are given by

$$\mathcal{F}_{j\rightarrow} = \sum_{l>j} \nabla U^{(2)}\left(q_j - q_l\right) \frac{p_j + p_l}{2}; \tag{6}$$

$\mathcal{F}_{j\rightarrow}$ describes the heat flow from the j^{th} to the l^{th} sites; $\mathcal{F}_{\rightarrow j}$ is obtained from the formula for $\mathcal{F}_{j\rightarrow}$ by changing l with j. It is useful to introduce the phase-space vector $\phi = (q,p)$ with $2N$ coordinates and write the equation for the dynamics (2) as

$$\dot{\phi} = -A\phi - {U^{(2)}}' + \sigma\eta, \tag{7}$$

where A and σ are $2N \times 2N$ matrices given by

$$A = \begin{pmatrix} 0 & -I \\ \mathcal{M} & \Gamma \end{pmatrix},\ \ \sigma = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{2\Gamma\mathcal{T}} \end{pmatrix}. \tag{8}$$

I above is the unit $N \times N$ matrix; and $\mathcal{M}$,Γ,$\mathcal{T}$ are diagonal $N \times N$ matrices: $\mathcal{M}_{jl} = M\delta_{jl}$, $\Gamma_{jl} = \zeta_j\delta_{jl}$, $\mathcal{T}_{jl} = T_j\delta_{jl}$. η are independent white-noises; ${U^{(2)}}'$ is the derivative of the $U^{(2)}$ term in H in relation to q (note that its contribution to $\dot{\phi}_k$ is nonzero only for $k > N$).

To study the dynamics we adopt the following strategy. First, we consider the system with $U^{(2)} = 0$, and stay with N independent sites connected, each one, to a heat bath. To recover the original dynamical system, we introduce the interaction among the sites and calculate the changes using techniques of stochastic differential equations. The solution of (7) above with $U^{(2)} \equiv 0$, is the Ornstein-Uhlenbeck process

$$\phi(t) = e^{-tA}\phi(0) + \int_0^t ds\ \ e^{-(t-s)A}\sigma\eta(s).$$

For simplicity we take $\phi(0) = 0$. The covariance of this Gaussian process is

$$\langle\phi(t)\phi(s)\rangle_0 \ \equiv\ \mathcal{C}(t,s) = \begin{cases} e^{-(t-s)A}\mathcal{C}(s,s) & t \geq s, \\ \mathcal{C}(t,t)e^{-(s-t)A^T} & t \leq s, \end{cases} \tag{9}$$
$$\mathcal{C}(t,t) = \int_0^t ds\ \ e^{-sA}\sigma^2 e^{-sA^T}.$$

From an easy computation (e.g. diagonalizing A), it follows that (for a single site ϕ_j)

$$\exp\left(-tA\right) = e^{-t\frac{\zeta_j}{2}}\cosh(t\rho_j)\left\{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right. \\ \left. + \frac{\tanh(t\rho_j)}{\rho_j}\begin{pmatrix} \frac{\zeta_j}{2} & 1 \\ -M & -\frac{\zeta_j}{2} \end{pmatrix}\right\}, \tag{10}$$

$\rho_j = \left((\zeta_j/2)^2 - M\right)^{1/2}$; the expressions for ϕ involving $2N \times 2N$ matrices are immediate. We assume that $\zeta_j/2,\quad M > 0$. If $(\zeta_j/2)^2 > M$, then ρ_j is real; otherwise, ρ_j is pure imaginary, but it does not spoil the dynamics: $\cosh(t\rho)$ in the formula above becomes $\cosh(t \cdot i\rho') = \cos(t\rho')$, etc. In this case (i.e., with $U^{(2)} = 0$), as $t \to \infty$ we have a convergence to equilibrium and the stationary state is Gaussian, with mean zero and covariance

$$C = \int_0^\infty ds\ \ e^{-sA}\sigma^2 e^{-sA^T} = \begin{pmatrix} \frac{\mathcal{T}}{M} & 0 \\ 0 & \mathcal{T} \end{pmatrix}, \tag{11}$$

where $\mathcal{T}$ is a diagonal matrix with elements $T_i\delta_{ij}$. To introduce the anharmonic coupling potential, we use the Girsanov theorem [14], which establishes a measure ν for the complete process (7) as an integral representation involving the measure $\mu_{\mathcal{C}}$ associated to the process without the potential $U^{(2)}$. Precisely, for any measurable set R, it states that $\rho(R) = E_0(1_R Z(t))$, where E_0 is the expectation for $\mu_{\mathcal{C}}$ (the measure for the process with $U^{(2)} = 0$); 1_R denotes the characteristic function, and

$$Z(t) = \exp\left(\int_0^t u\cdot dB - \tfrac{1}{2}\int_0^t u^2 ds\right); \\ \gamma_i^{1/2} u_i = -\nabla_{i-N} U^{(2)}; \tag{12}$$

the inner products above are in $\mathbb{R}^{2N}$ and ∇_k means the derivative in relation to ϕ_k. From (8) and the expression above for u_i, we have that u_i is nonvanishing only for $i > N$ (i.e., $i \in [N{+}1, N{+}2, \ldots, 2N]$). In what follows we will use the index notation: i for index values in the set $[N + 1, N+2, \ldots, 2N]$, j for values in the set $[1, 2, \ldots, N]$, and k for values in $[1, 2, \ldots, 2N]$. We will also be restricted to next-neighbor interactions, i.e., we take

$$U^{(2)} = \frac{1}{2}U^{(2)}(\phi_1 - \phi_2) + \frac{1}{2}U^{(2)}(\phi_{N-1} - \phi_N) + \\ + \sum_{j=2}^{N-1}\frac{1}{2}\left\{U^{(2)}(\phi_{j-1} - \phi_j) + U^{(2)}(\phi_j - \phi_{j+1})\right\},$$

where $U^{(2)}(x) = \lambda[1 - \cos(x)]$. Using the i, j, k index notation above, we may rewrite the stochastic equations for the decoupled process (where $U^{(2)} = 0$) as

$$d\phi_j = -A_{jk}\phi_k dt; \quad d\phi_i = -A_{ik}\phi_k dt + \gamma_i^{1/2} dB_i; \tag{13}$$

the sum over k (in $[1, 2 \ldots, 2N]$) is assumed above (as well as obvious sum over some indices in what follows).

Now, let us make explicit the terms in $Z(t)$. We have

$$u_i dB_i = \gamma_i^{-1/2} u_i \gamma_i^{-1/2} dB_i = -\gamma_i^{-1} U'_{i-N}\left(d\phi_i + A_{ik}\phi_k dt\right),$$

where we dropped out the upper index $^{(2)}$ in $U^{(2)}$ above (and in what follows); U'_{i-N} means the derivative in relation to ϕ_{i-N}, i.e., $U'_j = U'(\phi_j - \phi_{j+1}) - U'(\phi_{j-1} - \phi_j)$; $U'(\phi_j) = -\lambda\sin(\phi_j)$. From Itô formula [14], it follows that

$$\begin{gathered} -\left(U'_{j,j+1} - U'_{j-1,j}\right)\frac{d\phi_i}{\gamma_i} = -dF + \\ +\frac{\phi_i dt}{\gamma_i}\left(U''_{j,j+1}[\phi_{j+N} - \phi_{j+N+1}] - U''_{j,j-1}[\phi_{j+N-1} - \phi_{j+N}]\right), \\ F(\phi) = \gamma_i^{-1}\left(U'_{j,j+1} - U'_{j-1,j}\right)\phi_i, \end{gathered}$$

where $U'_{j,j+1} \equiv U'(\phi_j - \phi_{j+1})$, etc; and $j = i - N$ in the expressions above. Hence, we get

$$\begin{gathered} \int_0^t u_i dB_i = -\gamma_i^{-1}\Big([U'_{j,j+1} - U'_{j-1,j}][\phi_i(t) - \phi_i(0)] + \\ +\int_0^t \phi_i(s)[U''_{j,j+1}(\phi_i - \phi_{i+1}) - U''_{j-1,j}(\phi_{i-1} - \phi_i)](s)ds + \\ \int_0^t [U'_{j,j+1} - U'_{j-1,j}]A_{ik}\phi_k(s)ds\Big), \end{gathered} \tag{14}$$

and, for the u^2 term,

$$-\frac{1}{2}\int_0^t u_i^2 ds = -\frac{\gamma_i^{-1}}{2}\int_0^t [U'_{j,j+1} - U'_{j-1,j}]^2(s)ds, \tag{15}$$

where, again, $j = i - N$ an the sum over i (and so j) is assumed above. Then, for the correlation functions, we obtain an integral representation involving a "perturbative" potential and a Gaussian measure. E.g., for the two-point function we get $\langle\phi_k(t_1)\phi_q(t_2)\rangle = \mathcal{N}\int \phi_k(t_1)\phi_q(t_2)Z(t)d\mu_{\mathcal{C}}(\phi)$, $t_1, t_2 < t$; where $Z(t) = e^{-W}$, W is described by the several terms presented by the expressions above; $\mathcal{N}$ is the normalization.

The heat flow in the steady state is related to the formula (6). Precisely, for the case of next-neighbor interactions, the average over the stationary distribution for the current $\mathcal{F}_{v\to v+1}$ is obtained as the limit

$$\begin{gathered} \lim_{t\to\infty}\langle\mathcal{F}_{v\to v+1}\rangle = \lim_{t\to\infty} \\ \int [U'_{v,v+1}(\phi_u + \phi_{u+1})/2](t)Z(t)d\mu_{\mathcal{C}}(\phi) \Big/ \int Z(t)d\mu_{\mathcal{C}}(\phi)\ , \end{gathered}$$

where $v = u - N$ ($u > N$, obviously). Now, we carry out the computation. First note that $\mathcal{C}(t,s)$, given by (10)-(11), may be written as (for $t > s$) $\mathcal{C}(t,s) = \exp(-(t-s)A)C + \mathcal{O}\left(\exp[-(t+s)\zeta/2]\right)$, and the effects of the second term in the r.h.s of the equation above disappear in the correlation formula in the limit of $t\to\infty$ (recall that we must take this limit $t\to\infty$ in order to reach the steady state). Writing $Z(t) = e^{-\lambda W}$, the previous formula becomes

$$\lim_{t\to\infty}\langle\mathcal{F}_{v\to v+1}\rangle = \lim_{t\to\infty}\int \Omega e^{-\lambda W}d\mu_{\mathcal{C}}(\phi)\Big/\!\!\Big/\int e^{-\lambda W}d\mu_{\mathcal{C}}(\phi)\ ,$$

Ω given by the product of U' and ϕ described above. Up to first order in λ (i.e., for weak interaction between two sites), we have $\langle\mathcal{F}_{v\to v+1}\rangle = \langle\Omega\rangle_{\mathcal{C}} + \langle\Omega; -\lambda W\rangle_{\mathcal{C}}$, where $\langle\cdot\rangle_{\mathcal{C}}$ means the average in respect to $d\mu_{\mathcal{C}}$; $\langle\cdot;\cdot\rangle_{\mathcal{C}}$ means the truncated expectation. It is easy to see that $\langle\Omega\rangle_{\mathcal{C}}$ vanishes: U' depends on ϕ_v or ϕ_{v+1}, and $\langle\phi_v(t)\phi_u(t)\rangle_{\mathcal{C}} = \mathcal{C}_{v,u}(t,t) = 0$ (for any $v \le N$ and $u > N$). The terms in $-\lambda W$ are given by those describing $\int_0^t u_i dB_i$ (14), discarding that one involving $\phi(0)$ which vanishes in the computation as $t\to\infty$ ($\mathcal{C}(t,0)\to 0$ as $t\to\infty$). Note that we stay involved with expressions such as

$$\begin{gathered} \langle U'_{v,v+1}\phi_u(t); U'_{j,j+1}\phi_{\tilde{j}}(s)\rangle_{\mathcal{C}} = \\ -\frac{1}{4}\left\langle e^{i\phi_{v+1}(t)}e^{-i\phi_v(t)}\phi_u(t); e^{i\phi_{j+1}(s)}e^{-i\phi_j(s)}\phi_{\tilde{j}}(s)\right\rangle_{\mathcal{C}} + \ldots \end{gathered}$$

i.e., with integrals like $\int e^{i(h_1+\ldots+h_6)\cdot\phi}d\mu_{\mathcal{C}} - \int e^{i(h_1+h_2+h_3)\cdot\phi}d\mu_{\mathcal{C}}\int e^{i(h_4+h_5+h_6)\cdot\phi}d\mu_{\mathcal{C}}$, ($\phi_u(t)$ is obtained from $e^{ih\cdot\phi}$, obviously, by taking the derivative in relation to $h_u(t)$ and making $h\equiv 0$; the same for $\phi_{\tilde{j}}(s)$). After these integrations in ϕ, we get expressions such as

$$\lim_{t\to\infty}\int_0^t ds\ \mathcal{C}_{u,j+1}(t,s)\mathcal{C}_{v+1,\tilde{j}}(t,s)\exp[-\sum_{\alpha,\beta}\mathcal{C}_{\alpha,\beta}(t_\alpha,t_\beta)/2],$$

where t_α, t_β are t or s. For the case of small temperatures T_j, we have $\exp[\mathcal{C}_{\alpha,\beta}]\approx 1$. Thus, after all ϕ and s integrations (taking also the limit $t\to\infty$), we obtain

$$\mathcal{F}_{v\to v+1} = \frac{-\lambda^2}{2M(\zeta_v + \zeta_{v+1})}\left[\frac{\zeta_v}{\zeta_{v+1}}T_{v+1} - \frac{\zeta_{v+1}}{\zeta_v}T_v\right], \tag{16}$$

(to simplify the notation we write $\mathcal{F}_{v\to v+1}$ instead of $\lim_{t\to\infty}\langle\mathcal{F}_{v\to v+1}\rangle$). For the high temperature regime, we have to deal with expressions like $\lim_{t\to\infty}\int_0^t f(t,s)e^{-\theta g(t,s)}ds$, where $\theta\propto T$. We use the Laplace method [15] to get their asymptotic behavior $\theta\to\infty$. We obtain

$$\begin{aligned} \mathcal{F}_{v\to v+1} \approx\ & \frac{\lambda^2}{8}\left(\left(\frac{2}{\zeta_{v+1}} + \frac{1}{\zeta_{v+2}}\right)e^{-(T_{v+2}+T_v)/2M} - \left(\frac{2}{\zeta_v} + \frac{1}{\zeta_{v-1}}\right)e^{-(T_{v+1}+T_{v-1})/2M}\right) + \\ & + \frac{\lambda^2}{4(T_{v+1}+T_v)}\left[\left(\frac{T_{v+1}}{\zeta_{v+1}} - \frac{T_v}{\zeta_v}\right) - \left(\frac{T_{v+1}}{\zeta_v} - \frac{T_v}{\zeta_{v+1}}\right)\right]; \end{aligned} \tag{17}$$

with slight changes for the terms with $v = 1$ and $v = N$.

The steady state is characterized by $\langle dH_j/dt\rangle = 0$. Using this expression and also that $\lim_{t\to\infty}\langle\phi_i^2\rangle = T_{i-N}$ (taking the dominant contribution), which gives $\lim_{t\to\infty}\langle R_j(t)\rangle = 0$ for the interior sites j (i.e. the "self-consistent condition"), we have $\mathcal{F}_{1\to2} = \mathcal{F}_{2\to3} = \ldots = \mathcal{F}_{N-1\to N} \equiv \mathcal{F}$. Hence, for $\zeta_{j+1} - \zeta_j$ small, summing up $\mathcal{F}_{1\to2} + \mathcal{F}_{2\to3} + \ldots$ we obtain, for small temperatures,

$$\mathcal{F}\cdot 2M(\zeta_1 + 2\zeta_2 + \cdots + 2\zeta_{N-1} + \zeta_N) \approx \lambda^2(T_1 - T_N).$$

For uniform ζ, we have the Fourier's law

$$\mathcal{F} = \chi(T_1 - T_N)/(N-1), \qquad \chi = \lambda^2/4\zeta M.$$

As we make the inner couplings smaller and smaller we lose the factor N (which comes from $\zeta_2 + \ldots + \zeta_{N-1}$) and the Fourier's law does not hold anymore. For the case of high temperatures the sum of all $\mathcal{F}_{v\to v+1}$ gives us, for $\zeta_{v+1} - \zeta_v$ small,

$$\mathcal{F}(N-1) \approx \frac{\lambda^2}{4}\left(\frac{e^{-T_N/M}}{\zeta_N} - \frac{e^{-T_1/M}}{\zeta_1}\right),$$

which (essentially) does not depend on inner heat bath couplings, and so, the Fourier's law still holds when we make them smaller and smaller. Taking $\zeta_N = \zeta_1 = \zeta$, and $T_N = T_1 + \delta$ (δ small) the expression above becomes

$$\mathcal{F} \approx \frac{\lambda^2}{4M\zeta}e^{-T/M}\frac{(T_1 - T_N)}{(N-1)}, \tag{18}$$

where $e^{-T/M} = -[e^{-(T_1+\delta)/M} - e^{-T_1/M}]/[(T_1+\delta)/M - T_1/M]$, i.e., the conductivity decays exponentially at high temperatures, as in the rotor model [4]. Thus, still concerning the chain of rotators and the recent debate about the existence of a phase transition [11], [12], based on our results with cosine interactions, we believe in a divergent conductivity in low temperatures, as claimed in [12].

To argue about the reliability of our treatment, we recall some previous related works where the perturbative analysis gives the same result of the rigorous treatment. For the simpler case of the harmonic chain of oscillators with a bath at each site and identical next-neighbor interactions, a first order perturbative analysis [13] (for weak interactions, in a similar approach to that described here) gives the same result of the complete and rigorous treatment [9]. And following the procedures described here (analyzing different ζ_j), one may see that the perturbative result for this harmonic chain, in the limit of zero coupling between reservoirs and inner sites, will lead to the rigorous result obtained for the harmonic chain with thermal baths at the boundaries [2]. We still recall some previous works considering nonconservative stochastic Langevin systems (in contact with thermal reservoirs at the same temperature), but involving similar integral expressions for the correlations. There, the time decay of the two and/or four-point functions is detailed investigated in the regions of low and high temperatures. For the low temperature regime and weak interaction among the sites, we rigorously prove [16] that the complete treatment of the two and four-point functions adds only small corrections to the perturbative results [17]. For the same nonconservative system at high temperature, we developed a cluster expansion [18] which supports the perturbative analysis [19].

In short, in the present letter we develop an analytical method of modeling the heat conduction problem and study the heat current at the steady state of an anharmonic chain with weak interparticle (cosine) potential in order to investigate an old problem of heat conduction: may small anharmonic interactions lead to normal conductivity? We show that, if we keep the thermal reservoirs at the boundaries only, the Fourier's law holds for high but not for low temperatures.

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